

Benzenesulfonic acid, 3-hydrazino-
138-30-7 | DTXSID8059681

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.34

Global applicability domain: Inside

Local applicability domain index: 4.63e-01

Confidence level: 3.86e-01

Nearest Neighbors from the Training Set

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2,4-Diaminobenzenesulfonic acid

Measured: -4.65

Predicted: -2.19

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Benzamide, 2-bromo-6-nitro-

Measured: 0.28

Predicted: -0.0382

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p-Sulphamoylbenzamide

Measured: -0.830

Predicted: -0.618

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3-Sulfamoylbenzamide

Measured: -0.840

Predicted: -0.618